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catena-Poly[[tetraaquazinc(II)]-μ-2,2′-dihydroxy-5,5′-diazenediyldibenzoato]

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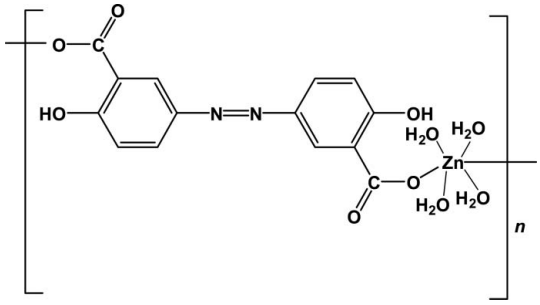
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.039; wR factor = 0.098; data-to-parameter ratio = 11.8.

In the title compound, $[Zn(C_{14}H_8N_2O_6)(H_2O)_4]_n$, the 2,2′-dihydroxy-5,5′-diazenediyldibenzoate ligand acts as a carboxylate bridge, leading to the formation of a polymeric chain running along the [1$\bar{1}$0] direction. The Zn^{II} atom is hexacoordinated in a distorted octahedral geometry by six O atoms [Zn—O = 2.055 (4)–2.132 (3) Å] from two carboxylate ligands and four water molecules. The crystal packing is stabilized by intermolecular O—H···O, O—H···N and C—H···O hydrogen bonds, and two π–π interactions. The centroid–centroid distances are 3.803 (16) and 3.804 (17) Å.

Related literature

For related literature, see: Klotz (2005); Tang, Tan & Cao (2007); Tang, Tan, Chen & Cao (2007); Tang, Yang *et al.* (2007).



Experimental

Crystal data

$[Zn(C_{14}H_8N_2O_6)(H_2O)_4]$
M_r = 437.66
Monoclinic, $P2_1/c$
a = 9.510 (2) Å
b = 11.255 (3) Å
c = 16.214 (4) Å
β = 107.019 (3)°
V = 1659.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.54 mm^{-1}
T = 296 (2) K
0.25 × 0.22 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.699, T_{max} = 0.861
10784 measured reflections
3278 independent reflections
3036 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.098
S = 1.10
3278 reflections
277 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O3*W*	2.055 (4)	Zn1—O2^{i}	2.086 (3)
Zn1—O4*W*	2.069 (4)	Zn1—O5	2.097 (3)
Zn1—O1*W*	2.075 (3)	Zn1—O2*W*	2.132 (3)
O3*W*—Zn1—O4*W*	177.75 (16)	O1*W*—Zn1—O5	94.52 (13)
O3*W*—Zn1—O1*W*	92.90 (16)	O2^{i}—Zn1—O5	85.89 (11)
O4*W*—Zn1—O1*W*	89.28 (15)	O3*W*—Zn1—O2*W*	88.49 (17)
O3*W*—Zn1—O2^{i}	89.72 (15)	O4*W*—Zn1—O2*W*	92.21 (18)
O4*W*—Zn1—O2^{i}	88.10 (14)	O1*W*—Zn1—O2*W*	86.44 (15)
O1*W*—Zn1—O2^{i}	177.36 (13)	O2^{i}—Zn1—O2*W*	93.32 (13)
O3*W*—Zn1—O5	87.93 (16)	O5—Zn1—O2*W*	176.33 (15)
O4*W*—Zn1—O5	91.35 (16)		

Symmetry code: (i) $x-1, y+1, z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O6	0.84 (6)	1.86 (6)	2.677 (5)	168 (6)
O1*W*—H1*WB*···N2^{ii}	0.88 (7)	2.32 (6)	3.058 (5)	143 (6)
O2*W*—H2*WA*···O1^{i}	1.01 (6)	1.63 (6)	2.636 (5)	170 (6)
O2*W*—H2*WB*···O3^{iii}	0.87 (7)	2.44 (8)	2.997 (5)	123 (6)
O3*W*—H3*WA*···N1^{iv}	0.74 (6)	2.17 (6)	2.893 (5)	164 (5)
O3*W*—H3*WB*···O6^{ii}	0.78 (8)	1.95 (7)	2.664 (5)	152 (7)
O4*W*—H4*WA*···O4^{v}	0.79 (7)	2.20 (8)	2.875 (6)	144 (8)
O4*W*—H4*WB*···O1^{ii}	0.89 (6)	1.85 (6)	2.703 (5)	160 (6)
O3—H3*A*···O2	0.82	1.80	2.528 (4)	147
O4—H4*A*···O5	0.82	1.81	2.537 (4)	148
C2—H2*A*···O1*W*^{vi}	0.93	2.53	3.405 (6)	157

Symmetry codes: (i) $x-1, y+1, z$; (ii) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x-1, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $-x+2, -y+1, -z$; (v) $-x+1, -y+1, -z$; (vi) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2258).

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supplementary materials

Acta Cryst. (2008). E**64**, m276-m277 [**doi:10.1107/S1600536807064860**]

catena-Poly[[tetraaquazinc(II)]-μ-2,2'-dihydroxy-5,5'-diazenediyldibenzoato]

Y.-H. Tan, Q.-S. Li, X.-P. Luo and X.-B. Xie

Comment

Olsalazine, 2,2'-dihydroxy-5,5'-diazenediyldibenzoic acid, has been widely used to prevent and treat the inflammatory bowel diseases, such as ulcerative colitis (Klotz, 2005). In previous work, we have synthesized a serial of Zn (Tang, Tan, Chen & Cao, 2007), Cd and Co (Tang, Yang *et al.*, 2007) complexes with phenanthroline as auxiliary ligand. We have also reported a Mn complex of olsalazine (Tang, Tan & Cao, 2007), but the zinc complex with single olsalazine as building block has not been reported yet. Here we reported the crystal structure of the title compound, (I), a new zinc complex of olsalazine.

In (I), the Zn atom is hexa-coordinated (Fig. 1) by two O atoms from two *L* ligands [H_2L=3,3-azo-bis(6-hydroxybenzoic acid)] and four water molecules in a distorted octahedral geometry (Table 1). Two ligands are *cis* to each other in an octahedral environment. Each ligand *L* acts as a carboxylate bridge, which leads to formation of a polymeric chain running in the direction [1$\bar{1}$0]. Two neighbouring polymeric chains are paired by π···π interactions between the aromatic rings; the distances *Cg*1···*Cg*1^{i} and *Cg*2···*Cg*2^{i} are 3.803 (16) and 3.804 (17) Å, respectively [*Cg*1 and *Cg*2 are centroids of C2—C7 and C8—C13 rings, respectively; symmetry code: (i) *x* - 1, *y* - 1, *z*]. The crystal packing is further stabilized by the intermolecular O—H···O, O—H···N and C—H···O hydrogen bonds (Table 2).

Refinement

The hydroxy and C-bound H atoms were placed in calculated positions (C—H = 0.93 Å and O—H = 0.82 Å) and included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C,*O*). The water H atoms were located in a difference Fourier map and refined isotropically.

Figures

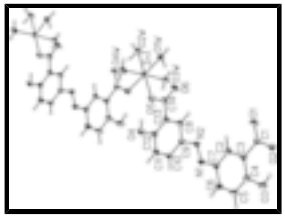

Fig. 1. A part of the polymeric structure of (I), showing displacement ellipsoids drawn at the 30% probability level and the atomic labelling. Unlabelled atoms are related to labelled atoms by the symmetry code (*x* - 1, *y* + 1, *z*).

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Crystal data

$[Zn(C_{14}H_8N_2O_6)(H_2O)_4]$	F_{000} = 896
M_r = 437.66	D_x = 1.752 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation

	λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 935 reflections
a = 9.510 (2) Å	θ = 1.8–26.0º
b = 11.255 (3) Å	μ = 1.54 mm^{-1}
c = 16.214 (4) Å	T = 296 (2) K
β = 107.019 (3)º	Block, orange
V = 1659.5 (7) Å^3	0.25 × 0.22 × 0.10 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3278 independent reflections
Radiation source: fine-focus sealed tube	3036 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 296(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	h = −11→11
T_{min} = 0.699, T_{max} = 0.861	k = −13→13
10784 measured reflections	l = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.098	$w = 1/[\sigma^2(F_o^2) + (0.0307P)^2 + 1.3308P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max} < 0.001$
3278 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
277 parameters	$\Delta\rho_{min}$ = −0.70 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.71408 (5)	0.64023 (4)	0.21196 (3)	0.03166 (13)
O6	0.9487 (4)	0.4284 (3)	0.2011 (2)	0.0620 (11)
O5	0.7705 (4)	0.5388 (3)	0.1179 (2)	0.0434 (8)
O4	0.6849 (4)	0.5057 (3)	−0.0439 (2)	0.0511 (9)
H4A	0.6873	0.5359	0.0025	0.077*
O3	1.5187 (4)	−0.2597 (3)	−0.0536 (2)	0.0570 (10)
H3A	1.5603	−0.2816	−0.0042	0.085*
O2	1.5791 (3)	−0.2637 (2)	0.10891 (19)	0.0375 (7)
O1	1.4725 (4)	−0.1395 (3)	0.17841 (18)	0.0508 (8)
O4W	0.5362 (4)	0.5313 (3)	0.2060 (3)	0.0535 (9)
O3W	0.8865 (4)	0.7510 (3)	0.2132 (3)	0.0501 (8)
O2W	0.6659 (4)	0.7520 (3)	0.3064 (2)	0.0493 (9)
O1W	0.8398 (4)	0.5403 (3)	0.3147 (2)	0.0431 (8)
N2	1.0930 (4)	0.1421 (3)	0.0030 (2)	0.0343 (7)
N1	1.1233 (4)	0.1052 (3)	−0.0637 (2)	0.0334 (8)
C14	0.8672 (5)	0.4557 (4)	0.1291 (3)	0.0402 (11)
C13	0.8783 (5)	0.3916 (3)	0.0511 (3)	0.0335 (9)
C12	0.7874 (5)	0.4192 (4)	−0.0312 (3)	0.0343 (9)
C11	0.7972 (5)	0.3553 (4)	−0.1026 (3)	0.0414 (10)
H11A	0.7367	0.3751	−0.1571	0.050*
C10	0.8949 (5)	0.2633 (4)	−0.0935 (3)	0.0372 (9)
H10A	0.8989	0.2196	−0.1414	0.045*
C9	0.9877 (5)	0.2357 (3)	−0.0127 (3)	0.0316 (9)
C8	0.9781 (5)	0.2998 (4)	0.0582 (3)	0.0370 (10)
H8A	1.0406	0.2807	0.1123	0.044*
C7	1.2236 (4)	0.0099 (3)	−0.0537 (3)	0.0322 (9)
C6	1.2416 (5)	−0.0349 (4)	−0.1298 (3)	0.0396 (10)
H6A	1.1871	−0.0025	−0.1822	0.048*
C5	1.3378 (6)	−0.1259 (4)	−0.1296 (3)	0.0473 (12)
H5A	1.3469	−0.1558	−0.1812	0.057*
C4	1.4210 (5)	−0.1727 (4)	−0.0517 (3)	0.0372 (10)
C3	1.4032 (4)	−0.1293 (4)	0.0259 (2)	0.0301 (8)
C2	1.3051 (5)	−0.0383 (3)	0.0244 (3)	0.0316 (9)
H2A	1.2936	−0.0093	0.0758	0.038*
C1	1.4901 (5)	−0.1794 (4)	0.1108 (3)	0.0321 (9)
H1WA	0.872 (6)	0.496 (5)	0.283 (4)	0.062 (18)*
H3WA	0.872 (7)	0.779 (5)	0.170 (4)	0.05 (2)*
H4WA	0.507 (9)	0.504 (6)	0.159 (5)	0.09 (3)*
H2WA	0.597 (7)	0.802 (5)	0.260 (4)	0.073 (19)*
H3WB	0.921 (7)	0.796 (6)	0.250 (5)	0.07 (2)*
H4WB	0.545 (7)	0.488 (5)	0.253 (4)	0.066 (19)*
H1WB	0.895 (8)	0.580 (6)	0.359 (4)	0.08 (2)*
H2WB	0.619 (8)	0.703 (6)	0.330 (5)	0.09 (3)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0368 (2)	0.0289 (2)	0.0260 (2)	0.0034 (2)	0.00388 (19)	0.0022 (2)
O6	0.076 (2)	0.070 (2)	0.0266 (18)	0.045 (2)	−0.0057 (17)	−0.0064 (16)
O5	0.0494 (18)	0.0396 (16)	0.0341 (18)	0.0196 (14)	0.0009 (13)	−0.0061 (13)
O4	0.056 (2)	0.0503 (18)	0.0372 (19)	0.0296 (16)	−0.0021 (15)	−0.0070 (15)
O3	0.076 (2)	0.062 (2)	0.0339 (19)	0.0451 (19)	0.0164 (18)	0.0057 (16)
O2	0.0453 (16)	0.0341 (14)	0.0297 (16)	0.0143 (13)	0.0057 (13)	0.0039 (12)
O1	0.068 (2)	0.0524 (16)	0.0286 (15)	0.0272 (18)	0.0085 (16)	0.0010 (16)
O4W	0.051 (2)	0.059 (2)	0.039 (2)	−0.0120 (16)	−0.0032 (17)	0.0131 (19)
O3W	0.060 (2)	0.055 (2)	0.030 (2)	−0.0195 (17)	0.0066 (17)	0.001 (2)
O2W	0.061 (2)	0.051 (2)	0.034 (2)	0.0169 (18)	0.0105 (16)	0.0009 (15)
O1W	0.0504 (19)	0.0440 (17)	0.0321 (19)	0.0105 (15)	0.0077 (14)	0.0042 (14)
N2	0.0380 (17)	0.0340 (15)	0.0279 (17)	0.0107 (16)	0.0052 (14)	0.0014 (16)
N1	0.0393 (18)	0.0326 (17)	0.0265 (18)	0.0100 (14)	0.0070 (15)	0.0019 (13)
C14	0.044 (2)	0.037 (2)	0.036 (3)	0.0115 (19)	0.0051 (19)	−0.0071 (19)
C13	0.039 (2)	0.0294 (19)	0.026 (2)	0.0077 (17)	−0.0003 (18)	−0.0018 (15)
C12	0.032 (2)	0.034 (2)	0.032 (2)	0.0076 (18)	0.0013 (16)	0.0019 (18)
C11	0.042 (2)	0.048 (2)	0.027 (2)	0.014 (2)	−0.0004 (18)	0.000 (2)
C10	0.047 (2)	0.039 (2)	0.023 (2)	0.0071 (19)	0.0049 (17)	−0.0056 (17)
C9	0.035 (2)	0.0302 (19)	0.028 (2)	0.0089 (16)	0.0061 (17)	−0.0002 (16)
C8	0.043 (2)	0.037 (2)	0.026 (2)	0.0108 (19)	0.0030 (18)	−0.0017 (18)
C7	0.035 (2)	0.0308 (19)	0.029 (2)	0.0071 (16)	0.0067 (17)	0.0030 (17)
C6	0.047 (3)	0.040 (2)	0.026 (2)	0.015 (2)	0.0027 (18)	0.0056 (18)
C5	0.068 (3)	0.049 (2)	0.023 (2)	0.020 (3)	0.009 (2)	−0.001 (2)
C4	0.046 (2)	0.034 (2)	0.031 (2)	0.0162 (18)	0.0108 (19)	0.0018 (17)
C3	0.035 (2)	0.0271 (17)	0.0262 (19)	0.0065 (17)	0.0064 (16)	0.0032 (17)
C2	0.035 (2)	0.0306 (19)	0.029 (2)	0.0051 (17)	0.0088 (17)	−0.0001 (17)
C1	0.036 (2)	0.0322 (19)	0.026 (2)	0.0039 (17)	0.0059 (17)	−0.0014 (16)

Geometric parameters (Å, °)

Zn1—O3W	2.055 (4)	N2—N1	1.267 (5)
Zn1—O4W	2.069 (4)	N2—C9	1.425 (5)
Zn1—O1W	2.075 (3)	N1—C7	1.413 (5)
Zn1—O2^{i}	2.086 (3)	C14—C13	1.487 (6)
Zn1—O5	2.097 (3)	C13—C8	1.385 (6)
Zn1—O2W	2.132 (3)	C13—C12	1.396 (6)
O6—C14	1.236 (6)	C12—C11	1.389 (6)
O5—C14	1.286 (5)	C11—C10	1.370 (6)
O4—C12	1.350 (5)	C11—H11A	0.9300
O4—H4A	0.8200	C10—C9	1.383 (6)
O3—C4	1.356 (5)	C10—H10A	0.9300
O3—H3A	0.8200	C9—C8	1.383 (6)
O2—C1	1.278 (5)	C8—H8A	0.9300
O2—Zn1^{ii}	2.086 (3)	C7—C2	1.387 (6)

O1—C1	1.240 (5)	C7—C6	1.389 (6)
O4W—H4WA	0.80 (8)	C6—C5	1.372 (6)
O4W—H4WB	0.88 (7)	C6—H6A	0.9300
O3W—H3WA	0.74 (6)	C5—C4	1.382 (6)
O3W—H3WB	0.78 (7)	C5—H5A	0.9300
O2W—H2WA	1.02 (7)	C4—C3	1.406 (6)
O2W—H2WB	0.87 (7)	C3—C2	1.381 (5)
O1W—H1WA	0.83 (6)	C3—C1	1.493 (5)
O1W—H1WB	0.88 (7)	C2—H2A	0.9300
O3W—Zn1—O4W	177.75 (16)	C12—C13—C14	121.8 (4)
O3W—Zn1—O1W	92.90 (16)	O4—C12—C11	117.9 (4)
O4W—Zn1—O1W	89.28 (15)	O4—C12—C13	121.6 (4)
O3W—Zn1—O2^{i}	89.72 (15)	C11—C12—C13	120.5 (4)
O4W—Zn1—O2^{i}	88.10 (14)	C10—C11—C12	120.7 (4)
O1W—Zn1—O2^{i}	177.36 (13)	C10—C11—H11A	119.7
O3W—Zn1—O5	87.93 (16)	C12—C11—H11A	119.7
O4W—Zn1—O5	91.35 (16)	C11—C10—C9	119.8 (4)
O1W—Zn1—O5	94.52 (13)	C11—C10—H10A	120.1
O2^{i}—Zn1—O5	85.89 (11)	C9—C10—H10A	120.1
O3W—Zn1—O2W	88.49 (17)	C8—C9—C10	119.4 (4)
O4W—Zn1—O2W	92.21 (18)	C8—C9—N2	116.8 (4)
O1W—Zn1—O2W	86.44 (15)	C10—C9—N2	123.8 (4)
O2^{i}—Zn1—O2W	93.32 (13)	C9—C8—C13	122.0 (4)
O5—Zn1—O2W	176.33 (15)	C9—C8—H8A	119.0
C14—O5—Zn1	128.2 (3)	C13—C8—H8A	119.0
C12—O4—H4A	109.5	C2—C7—C6	119.2 (4)
C4—O3—H3A	109.5	C2—C7—N1	125.4 (4)
C1—O2—Zn1^{ii}	128.5 (3)	C6—C7—N1	115.4 (3)
Zn1—O4W—H4WA	109 (6)	C5—C6—C7	121.6 (4)
Zn1—O4W—H4WB	114 (4)	C5—C6—H6A	119.2
H4WA—O4W—H4WB	122 (6)	C7—C6—H6A	119.2
Zn1—O3W—H3WA	109 (5)	C6—C5—C4	119.3 (4)
Zn1—O3W—H3WB	125 (5)	C6—C5—H5A	120.3
H3WA—O3W—H3WB	111 (7)	C4—C5—H5A	120.3
Zn1—O2W—H2WA	91 (3)	O3—C4—C5	117.9 (4)
Zn1—O2W—H2WB	101 (5)	O3—C4—C3	122.2 (4)
H2WA—O2W—H2WB	112 (5)	C5—C4—C3	119.9 (4)
Zn1—O1W—H1WA	93 (4)	C2—C3—C4	120.0 (3)
Zn1—O1W—H1WB	117 (4)	C2—C3—C1	119.0 (4)
H1WA—O1W—H1WB	125 (6)	C4—C3—C1	121.0 (4)
N1—N2—C9	114.4 (3)	C3—C2—C7	120.0 (4)
N2—N1—C7	117.7 (3)	C3—C2—H2A	120.0
O6—C14—O5	122.6 (4)	C7—C2—H2A	120.0
O6—C14—C13	120.1 (4)	O1—C1—O2	123.5 (4)
O5—C14—C13	117.3 (4)	O1—C1—C3	119.8 (4)
C8—C13—C12	117.6 (4)	O2—C1—C3	116.7 (4)
C8—C13—C14	120.6 (4)		

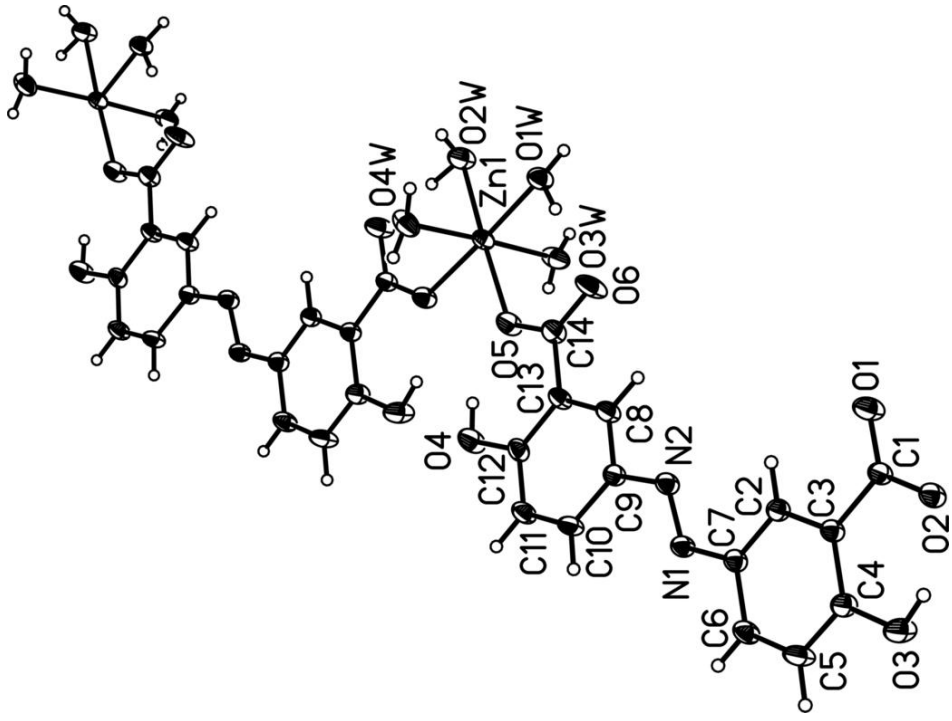
Symmetry codes: (i) *x*−1, *y*+1, *z*; (ii) *x*+1, *y*−1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O6	0.84 (6)	1.86 (6)	2.677 (5)	168 (6)
O1W—H1WB···N2^{iii}	0.88 (7)	2.32 (6)	3.058 (5)	143 (6)
O2W—H2WA···O1^{i}	1.01 (6)	1.63 (6)	2.636 (5)	170 (6)
O2W—H2WB···O3^{iv}	0.87 (7)	2.44 (8)	2.997 (5)	123 (6)
O3W—H3WA···N1^{v}	0.74 (6)	2.17 (6)	2.893 (5)	164 (5)
O3W—H3WB···O6^{iii}	0.78 (8)	1.95 (7)	2.664 (5)	152 (7)
O4W—H4WA···O4^{vi}	0.79 (7)	2.20 (8)	2.875 (6)	144 (8)
O4W—H4WB···O1^{iii}	0.89 (6)	1.85 (6)	2.703 (5)	160 (6)
O3—H3A···O2	0.82	1.80	2.528 (4)	147
O4—H4A···O5	0.82	1.81	2.537 (4)	148
C2—H2A···O1W^{vii}	0.93	2.53	3.405 (6)	157

Symmetry codes: (iii) −*x*+2, *y*+1/2, −*z*+1/2; (i) *x*−1, *y*+1, *z*; (iv) *x*−1, −*y*+1/2, *z*+1/2; (v) −*x*+2, −*y*+1, −*z*; (vi) −*x*+1, −*y*+1, −*z*; (vii) −*x*+2, *y*−1/2, −*z*+1/2.

Fig. 1


O4W
O2W
Zn1
O1W
O3W
O6
O5
C14
C13
C8
O4
C12
N2
C11
C9
C10
C7
C2
C3
O1
C1
O2
N1
C4
C6
O3
C5